John von Neumann Institute for Computing

DEISA: Enabling Cooperative Extreme Computing in Europe

Hermann Lederer, Victor Alessandrini

published in

Parallel Computing: Architectures, Algorithms and Applications ,
C. Bischof, M. Bücker, P. Gibbon, G.R. Joubert, T. Lippert, B. Mohr, F. Peters (Eds.),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **38**, ISBN 978-3-9810843-4-4, pp. 689-696, 2007.
Reprinted in: Advances in Parallel Computing, Volume **15**,
ISSN 0927-5452, ISBN 978-1-58603-796-3 (IOS Press), 2008.

http://www.fz-juelich.de/nic-series/volume38

DEISA: Enabling Cooperative Extreme Computing in Europe

Hermann Lederer[1] **and Victor Alessandrini**[2]

[1] Rechenzentrum Garching der Max-Planck-Gesellschaft
Boltzmannstr. 2, D-85748 Garching, Germany
E-mail: Lederer@rzg.mpg.de

[2] CNRS/IDRIS, Bâtiment 506, BP 167
91403 Orsay cedex, France
E-mail: va@idris.fr

The DEISA European Research Infrastructure has been designed to act as a vector of integration of High Performance Computing (HPC) resources at the continental scale. Its services have been tailored to enable seamless access to, and high performance cooperative operation of, a distributed park of leading supercomputing platforms in Europe. The DEISA services are deployed on top of a dedicated high speed network infrastructure connecting computing platforms, using selected middleware. Their primordial objective is enabling capability computing across remote computing platforms and data repositories. Workflows across different platforms, transparent remote I/O, and large file transfers are starting to operate without inducing performance bottlenecks that would invalidate high performance computing. These services will bloom as the number of scientific users accessing different computing platforms in Europe will grow. After reviewing the existing services and the DEISA research Infrastructure based today on the DEISA Extreme Computing Initiative, we discuss how DEISA has been paving the way to the deployment of a coherent HPC environment in Europe, and why their persistency is mandatory to support and cooperate with new initiatives like PRACE in the area of HPC. Some comments are advanced about the relevance of the DEISA environment for the efficient operation of future European supercomputers, and the current vision about the overall role of DEISA in the new emerging European HPC ecosystem is discussed.

1 DEISA — The Origin

In early 2002 the idea was born to overcome the fragmentation of supercomputing resources in Europe both in terms of system availability and in the necessary skills for efficient supercomputing support. After an Expression of Interest to the EU in Spring 2002 proposing to establish a distributed European supercomputing infrastructure, the DEISA project was started in May 2004 as a EU FP6 Integrated Infrastructure Initiative by eight leading European supercomputing centres and expanded in 2006 by three additional leading centres. DEISA — the Distributed European Infrastructure for Supercomputing Applications[1], is now in its fourth year since starting the deployment of the infrastructure, has reached production quality to support leading edge capability computing for the European scientific community.

2 The Consortium

The DEISA Consortium is constituted from eleven partners from seven European countries: BSC, Barcelona (Spain); CINECA, Bologna (Italy); CSC, Espoo (Finland); EPC-

C/HPCx, Edinburgh and Daresbury (UK); ECMWF, Reading (UK); FZJ, Jülich (Germany); HLRS, Stuttgart (Germany); IDRIS-CNRS, Orsay (France); LRZ, Munich/Garching (Germany); RZG, Garching (Germany); and SARA, Amsterdam (The Netherlands).

3 Key Features of DEISA

The guiding strategy of the DEISA Consortium has been the integration of national supercomputing systems using selected Grid technologies, to add value to the existing environments and to provide an extra layer of European HPC services on top of them. The DEISA Consortium has used Grid technologies to enhance HPC in Europe and take the first steps towards the creation of a European HPC ecosystem. Outstanding features of the integrated infrastructure are:

- High speed end-to-end network
- Common global high performance file system at continental scale to greatly facilitate data management across Europe
- Uniform infrastructure access through the UNICORE middleware system
- Harmonization of the manifold heterogeneous software environments through the DEISA Common Production Environment DCPE
- Portals and internet interfaces for transparent access to complex supercomputing environments
- Job re-routing across Europe
- Joint research activities in major scientific disciplines
- Enabling of cooperative Extreme Computing in Europe

3.1 High speed end-to-end network

National supercomputers have been tightly interconnected by a dedicated high performance network infrastructure provided by GÉANT2 and the National Research Network providers (NREN). As illustrated in Fig. 1, the network backbone is based today on 10 Gbit/s technology.

3.2 Common global high performance file system at continental scale

High performance wide-area global file systems such as GPFS from IBM open up totally new modes of operation within grid infrastructures, especially in supercomputing grids with a fairly limited number of participating sites. A common data repository with fast access, transparently accessible both by applications running anywhere in the grid, and by scientists working at any partner site as entry point to the grid, greatly facilitates cooperative scientific work at the continually increasing geographically distributed scientific communities. During the Supercomputing Conference 2005, a supercomputing hyper-grid

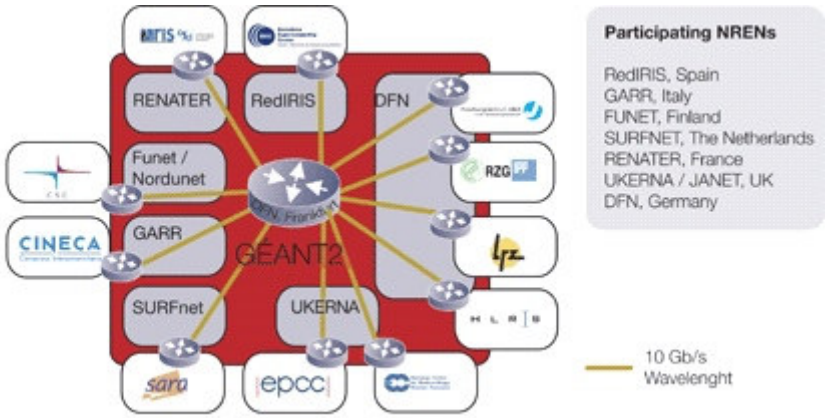

Figure 1. DEISA dedicated network based on 10 Gbit/s technology provided by GÉANT2 and the NRENs

was created to move a step towards interoperability of leading grids. A dedicated network connection was established between DEISA and TeraGrid[2], and the DEISA and TeraGrid global file systems were interconnected to build a huge, global file system spanning two continents [3 4 5].

3.3 Uniform infrastructure access through the UNICORE middleware system

The UNICORE middleware[6] is *the* main gateway to DEISA. It facilitates end-user instrumentation, provides secure access to distributed compute resources, enables single sign-on and provides a graphical user interface to batch-subsystems and to file systems. And UNICORE greatly facilitates the set-up of complex workflows[7 8]. A command line tool is available via the DEISA Services for the Heterogeneous management Layer, or DESHL, which permits the user to manage their DEISA jobs directly from their workstation.

3.4 Harmonization of the manifold heterogeneous software environments

The DEISA supercomputing infrastructure is characterized by a large diversity of HPC architectures with heterogeneous software environments. Architectures include today systems based on Power4, Power4+, and Power5 processors from IBM in various node sizes, running the operating system AIX, Power5+ and PowerPC from IBM running Linux, SGI Altix 4700 from SGI with Intel IA64 Itanium2/Montecito processors running Linux, Cray XT4 from Cray with AMD Opteron processors running Linux, NEC SX-8 vector system running Super UX.

Application and user support specialists have therefore developed the DEISA Common Production Environment (DCPE), to provide a uniform DEISA environment for the users, with the same appearance and functionality, whatever the underlying architecture: homogeneous access to the heterogeneous supercomputing cluster. Details are given in the DEISA Primer[9].

3.5 Science gateways

Infrastructure access for the Life Science and Materials Science communities has additionally been facilitated by specific science gateways, completely hiding the complexity of the distributed infrastructure and providing application-specific enhancements[10] [11].

3.6 Job re-routing across Europe

Job re-routing across Europe has been put into place among five platforms with the same operating system to a) free resources for a big job requiring close to all resources at one site, and b) to facilitate simultaneous usage of many platforms for independent subtasks of a big project, to accelerate project turn-around in a complementary approach to using UNICORE.

3.7 Joint Research Activities in major scientific disciplines

Joint Research Activities (JRAs) have been carried out to closely work with early adopters of the infrastructure from different scientific communities to address specific needs, e.g. from Materials Science, Cosmology, Plasma Physics, Life Sciences, and Engineering & Industry. As an example, the JRA in plasma physics has supported EFDA[12] in adhoc and expert groups for HPC and has addressed the enabling and optimization of the majority of the European turbulence simulation codes considered by EFDA as highly relevant for ITER[13].

3.8 Extreme Computing and Applications Enabling in Europe

Of key importance for an adequate usability of state-of-the-art and next generation supercomputers is applications enabling. A team of leading experts in high performance and Grid computing, the so-called Applications Task Force, provides application support in all areas of science and technology. In 2005 the DEISA Extreme Computing Initiative (DECI) was launched for the support of challenging computational science projects. One of the key tasks is hyperscaling, a unique service not offered by any other European grid computing project. Hyperscaling aims at application enabling towards efficient use of thousands or tens of thousands of processors for the same problem, a prerequisite for applications to benefit from forthcoming Petaflop scale supercomputers.

Application and user support specialists have enabled and optimized applications for usage in DEISA. Two European plasma physics simulation codes, GENE and ORB5, have been scaled up to 8000 processor-cores and beyond[14]. Examples of application enabling in addition to hyperscaling include: design of coupled applications; determination of best suited architecture(s) in DEISA; adaptation of applications to the DEISA infrastructure and architecture dependent optimizations.

Since late 2005, DEISA has been used for conducting the most challenging European projects in computational sciences requiring the most advanced supercomputing resources available through DEISA. Over 50 projects from the 2005 and 2006 DECI calls have already benefited from the Extreme Computing Initiative. Close to thirty papers have already been published upon DECI projects. Examples of very successful projects include:

Figure 2. Cover page of Nature (May 24, 2007) referring to the results of the DECI project POLYRES[15]

POLYRES (German/British group, Principal Investigator (P.I.) Kurt Kremer): Water & Salt, Fluid Membranes. For almost two decades, physicists have been on the track of membrane mediated interactions. Simulations in DEISA have now revealed that curvy membranes make proteins attractive, reported as cover story of NATURE[15] (see Fig. 2).

BET (Italian/Swiss/British consortium, P.I. Paolo Carloni): First-Principles and Mixed quantum classical QM/MM Simulations of Biological Electron Transfer. The study showed that full ab initio calculations on bio-molecules at physiological conditions are now possible by exploiting modern quantum chemistry protocols and today's large-scale supercomputing facilities, like those made available through the DEISA initiative[16 17].

CAMP (Swiss/Hungarian group, P.I. Michele Parrinello): Catalysis by Ab-initio Metadynamics in Parallel. Pyrite has been suggested as the key catalyst in the synthesis of prebiotic molecules under anoxic conditions in the early history of the Earth. A better understanding of the pyrite surface and its chemistry was achieved by means of ab-initio calculations[18 19].

GIMIC: The international VIRGO Consortium (http://www.virgo.dur.ac.uk, P.I.'s Simon White and Carlos Frenk) have performed the Galaxies-Intergalactic Medium Interaction Calculation. The results of the cosmological simulations are illustrated in Fig. 3

In the third successful year of the DECI, over 60 proposals were received from the 2007 call, requesting a total of more than 70 million processor hours. Since multi-national proposals are especially encouraged by DEISA, scientists from 15 different European countries have so far been involved in DECI, some with partners from other continents: namely North and South America, Asia and Australia.

4 Conclusions

The DEISA Consortium has contributed to raising awareness of the need for a European HPC ecosystem. Since its formation in 2002, the consortium has directed its efforts towards the integration of leading national supercomputing resources on a continental scale. Its fundamental objective has been the deployment and operation of a distributed Euro-

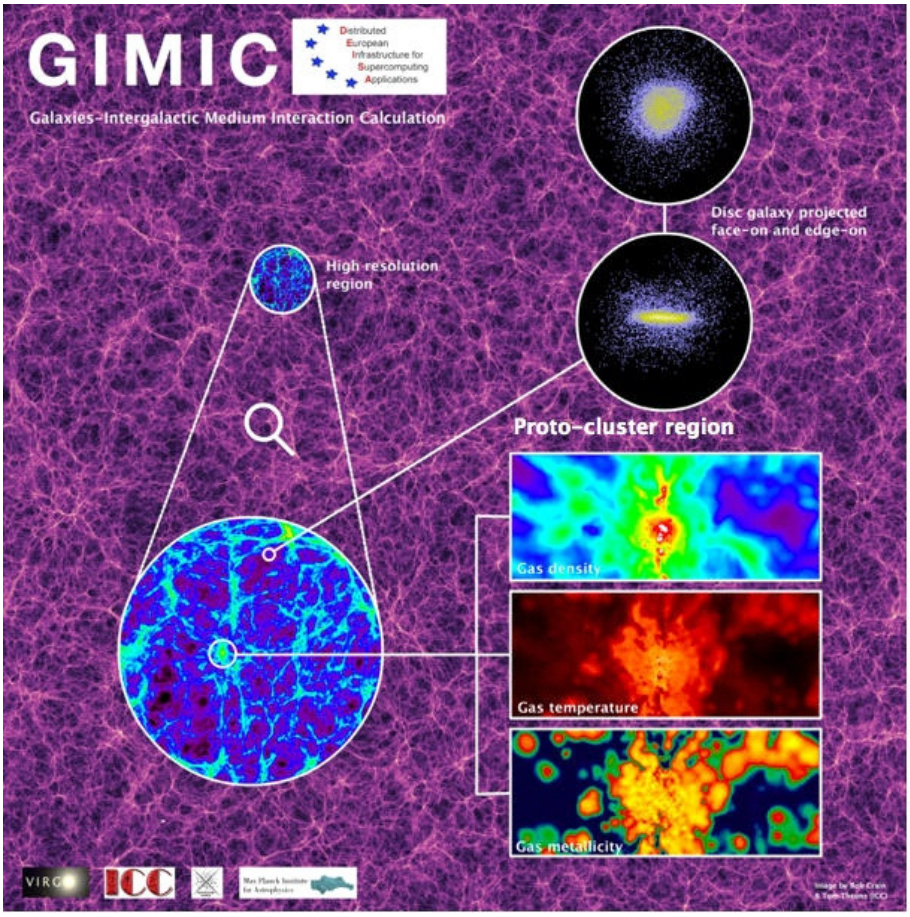

Figure 3. Illustration of the results of the GIMIC DECI project of the international VIRGO Consortium, simulating Galaxies-Intergalactic Medium Interaction Calculation

pean HPC environment capable of enabling the high performance cooperative operation of a number of leading national supercomputing systems in Europe, thereby drawing international attention to Europe's rising international competitiveness in the HPC area. The importance of a European HPC ecosystem was recognised in the ESFRI. DEISA has paved the way to provide the operational infrastructure for the forthcoming shared European supercomputing platforms that are the target of new initiatives in Europe (PRACE) today. DEISA is advancing computational sciences in Europe and has increased Europe's visibility in the supercomputing domain.

Acknowledgements

The DEISA Consortium thanks the European Commission for support through contracts FP6-508830 and FP6-031513.

References

1. Distributed European Infrastructure for Supercomputing Applications (DEISA), http://www.deisa.org
2. TeraGrid http://www.teragrid.org
3. http://cordis.europa.eu/ictresults/index.cfm/section/news/tpl/article/BrowsingType/-Features/ID/80183
4. P. Andrews, C. Jordan and H. Lederer, *Design, implementation, and production experiences of a global storage grid*, in: *Proc. 14th NASA Goddard, 23rd IEEE Conference on Mass Storage Systems and Technologies*, (2006).
5. P. Andrews, M. Buechli, R. Harkness, R. Hatzky, C. Jordan, H. Lederer, R. Niederberger, A. Rimovsky, A. Schott, T. Soddemann and V. Springel, *Exploring the hypergrid idea with grand challenge applications: The DEISA- TeraGrid interoperability demonstration*, in: *Challenges of Large Applications in Distributed Environments, 2006 IEEE*, pp. 43–52, (2006).
6. UNICORE http://www.unicore.org
7. L. Clementi, M. Rambadt, R. Menday and J. Reetz, *UNICORE Deployment within the DEISA Supercomputing Grid Infrastructure*, *Proc. 2nd UNICORE Summit 2006 in conjunction with EuroPar 2006 Dresden, Germany*, LNCS **4375**, pp. 264–273, (2006).
8. M. Rambadt, R. Breu, L. Clementi, Th. Fieseler, A. Giesler, W. Gürich, P. Malfetti, R. Menday, J. Reetz and A. Streit, *DEISA and D-Grid: using UNICORE in production Grid infrastructures*, *Proc. German e-Science Conference 2007, Baden-Baden*, Max Planck Digital Library, ID 316544.0, (2007).
9. DEISA Primer http://www.deisa.org/userscorner/primer
10. T. Soddemann, *Science gateways to DEISA*, in: Concurrency Computat. Pract. Exper., DOI 10.1002/cpe, (2006).
11. T. Soddemann, *Job management enterprise application*, in: W. Lehner et al. (eds): Euro-Par 2006 Workshops, Lecture Notes in Computer Science **4375**, pp. 254–263, (2007)
12. European Fusion Development Agreement EDFA. http://www.efda.org
13. ITER http://www.iter.org
14. H. Lederer, R. Hatzky, R. Tisma and F. Jenko, *Hyperscaling of plasma turbulence simulations in DEISA*, *Proc. 5th IEEE workshop on Challenges of large applications in distributed environments*, p. 19, (ACM Press, New York, 2007).
15. B.J. Reynwar, G. Illya, V.A. Harmandaris, M.M. Müller, K. Kremer and M. Deserno, *Aggregation and vesiculation of membrane proteins, by curvature mediated interactions*, Nature, **447**, doi:10.1038/nature05840, (2007).
16. M. Cascella, A. Magistrato, I. Tavernelli, P. Carloni and U. Rothlisberger, *Role of protein frame and solvent for the redox properties of azurin from Pseudomonas aeruginosa Cascella*, *Proc. National Academy of Sciences of the United States of America*, **103**, pp. 19641–19646, (2006).
17. M. Sulpizi, S. Raugei, J. VandeVondele, M. Sprik and P. Carloni, *Calculation of redox properties: understanding short and long range effects in rubredoxin*, J. Phys. Chem. B, **111**, 3969–3976, (2007).
18. A. Stirling, M. Bernasconi and M. Parrinello, *Defective pyrite (100) surface: An ab*

initio study, Phys. Rev. B, **75**, 165406, (2007).
19. T. D. Kuehne, M. Krack, F. R. Mohamed and M. Parrinello, *Efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer molecular dynamics*, Phys. Rev. Lett., **98**, 066401, (2007).